Preparation and Characterization of MoO_3 as an hole-transporting layer (HTL) in organic Photovoltaic's.

Kamal Solanki[1],Shilpa Sharma[*], D.N. Dewangan[2]

1. *Assistant Professor,Rungta College of Engineering & Technology, Raipur, Chhattisgarh.*
2. *Principal, Rungta College of Engineering & Technology, Raipur, Chhattisgarh*

** Associate Professor, Rungta College of Engineering & Technology, Raipur, Chhattisgarh*

Abstract

In this work, the preparation of Molybdenum solution using Ethanediol and Isopropanol as solvent by an ultrasonic reaction was done. The favorably smooth and dense surface morphology of the s-MoO3 layers are obtained under 200 °C thermal treatment with the help of hydrothermal method. The structural, electronic properties of the s-MoO_3 thin film are investigated in by UV- Visible spectroscopy. The results indicate that the s-MoO3 thin film possesses appropriate morphological, optical and electronic properties to be suitable for organic photovoltaic applications. The photovoltaic devices have been investigated and optimized in detail by tuning layer thickness, processing temperature and time, annealing conditions of interfacial layers.

1. Introduction

In current era the development of bulk heterojunction (BHJ) polymer solar cells (PSCs) continues to show progress, polymer solar cell is really a cost effective so in the upcoming year it's a relatively a best research topic. A BHJ polymer solar cell generally consists of a transparent anode (typically indium tin oxide, ITO/fluorine doped tin oxide FTO), a BHJ active layer (a mixture of donor polymer a fullerene acceptor), and a cathode (e.g. Ag/Al). Anode and cathode play a very important role in organic solar cell for charge collection. The development of hole and electron transport or the blocking layers are usually play a very important role for efficient charge transfer in a device and also play a very important role in reducing the chances of recombination of the charges in the devices. Now a days the aqueous poly (3, 4- ethylenedioxythiophene) poly (styrene sulfonate) (PEDOT: PSS) is typically used as the Hole transport layer in the polymer solar cell. However, PEDOT : PSS has the typically nature of absorbing moisture from air so due to this the stability factor is not so good, to avoid these problems, In this work the most stable hole transport layer is used to make the solar cell more effective .In this regard transition metal oxide semiconductors including NiO, MoO_3 V_2O_5 and WO_3 are emerging as a best candidates of substitutes for PEDOT:PSS as the hole-transporting layer (HTL), which is having high transmittance in the visible range which can be easily demonstrated by UV-visible spectrophotometer Moreover, the molybdenum solution s low cost easily prepared in the lab[1].

Organic photovoltaics (OPVs) based on organic polymers and small molecules have attracted increasing attentions over the past decades as the potential low-cost alternatives to silicon-based solar cells [1–5]. As the efficiency and stability of the OPV devices improve progressively with structure optimization of new photoactive and interfacial materials, the field is approaching efficiently manufacturable technologies [6–11]. Compared to bilayer devices configuration, bulk heterojuction (BHJ) structure is using an intimate blend of electron donor (D) and electron acceptor (A) materials to build up self-assembling nanoscale interpenetrating network and phase-separated domains in nanometer level, which can be introduced using various film deposition technologies such as spray coating, spin-casting, roll-to-roll processing and inkjet printing [12,13]. This architecture has a significant advantage in that a great proportion of the excitons are within the diffusion length of a D–A interface (about 5–10 nm) [14,15]. However an inherent limitation of the BHJ architecture is that the active layer materials can directly contact with both anode (generally indium tin oxide (ITO)) and cathode (e.g., Ca, Al), which creating an environment that risks significant minority carrier collection.

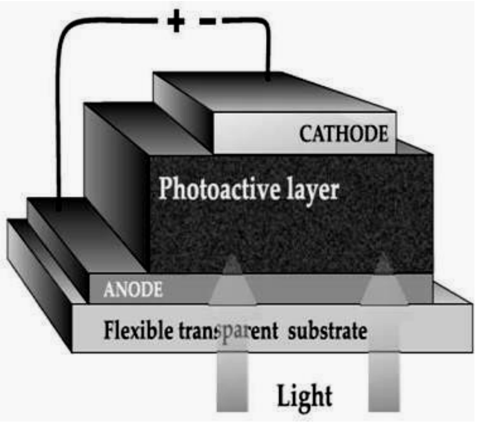

Figure 1. Organic Solar Cell

Bulk-Heterojunction solar cell: Bulk heterojunctions are most commonly created by forming a solution containing the two components, casting (e.g. drop casting and spin coating) and then allowing the two phases to separate, usually with the assistance of an annealing step. The two components will self- assembles into an interpenetrating network connecting the two electrodes. They are normally composed of a conjugated molecule based donor and fullerene based acceptor. The nanostructure morphology of bulk heterojunctions tends to be difficult to control, but is critical to photovoltaic performance. After the capture of a photon, electrons move to the acceptor domains, then are carried through the device and collected by one electrode, and holes move in the opposite direction and collected at the other side. If the dispersion of the two materials is too fine, it will result in poor charge transfer through the layer.

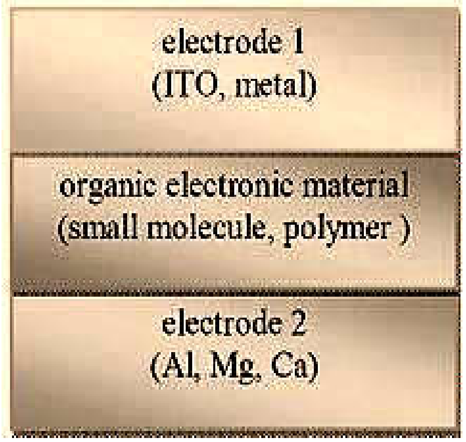

Figure 2. Single layer Organic Solar Cell

2. Experiment

2.1. Reagents and materials

Indium tin oxide (ITO) coated glass substrates were purchased from CSG HOLDING CO., Ltd. (China). Ethylene glycol , Isopropyl alcohol and Hydrogen peroxide were purchased from MOLYCHEM Chemical Reagent Co., Ltd. Electron donor material P3HT and electron acceptor material PC61BM were purchased from Luminescence Technology Corp

2.2 Preparation of the molybdenum solution

The synthesis was based on the preparation of perexomolybdic acid solution with the treatment of ultrasonic reaction. Firstly the ethanediol and isopropanol were generally mixed in order to obtain the 40ml complex solvent by the volume ratio of (1:9)(ethanediol to isopropanol). Then the MoO_3 powder (400mg) mixed with the complex solvent. Then 30% aqueous H_2O_2 were added to the reacted system by volume ratio (7:93). Then the total solution was ultrasonication for around 30 minutes. At last, the thermal treatment 200c provided with the help of hydrothermal method

2.3 Instrumentation

SEM imaging was conducted on S-4800 scanning electron microscope operated at an acceleration voltage of 4 kV. AFM was used to measure film roughness and surface morphologies in tapping mode using a Veeco dimension V atomic microscope at room temperature. The AFM cantilever coated with Pt/Ir was employed for conductive-AFM measurement and contact mode was selected while applying a þ10 mV bias. The transmittance spectra were recorded on a ELICO SL 159UV-VISIBLE Spectrophotometer.

3. Results and Discussion

3.1 Optical property of molybdenum solution:

ELICO SL 159UV-VISIBLE Spectrophotometer was used for the measurement of the ultraviolet and visible spectra of the solution. So, Firstly the UV-VISIBLE measurement was carried on the molybdenum solution in the room temperature as well in 200 degree centigrade .However a growing small broad spectra ranging from 600nm to 800nm is absorbed for the annealing temperature 200 degree centigrade and due to high annealing temperature the small broad spectra becomes more evident and this fascinating phenomenon may be attributed to the free electron being trapped in the oxygen vacancies in these p-moo3 which result in hole transport layer as well as Electron Blocking layer. The transmission spectrum of Molybdenum solution almost covers entire spectrum of visible wavelength which is really wonderful, so that the entire visible spectrum transmitted to active layer [2].

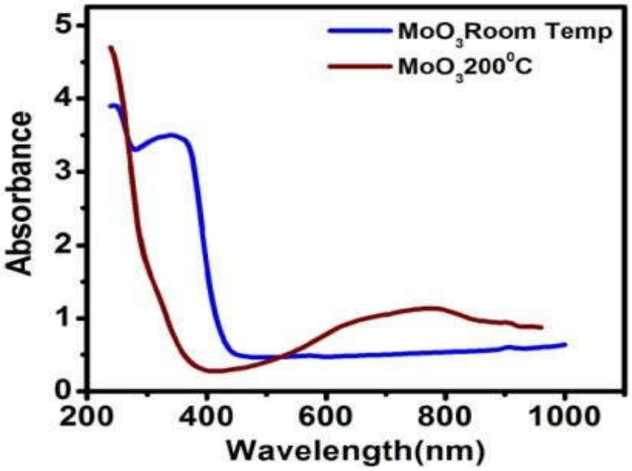

Figure 3.1: UV-visible absorption spectra of the MoO3 under room temperature and at 200 degree centigrade.

Optical property of PEDOT: PSS solution- The UV-VISIBLE measurement was carried on the PEDOT: PSS solution in the room temperature. The Transmittance spectra of PEDOT: PSS Solution was shown in the figure.

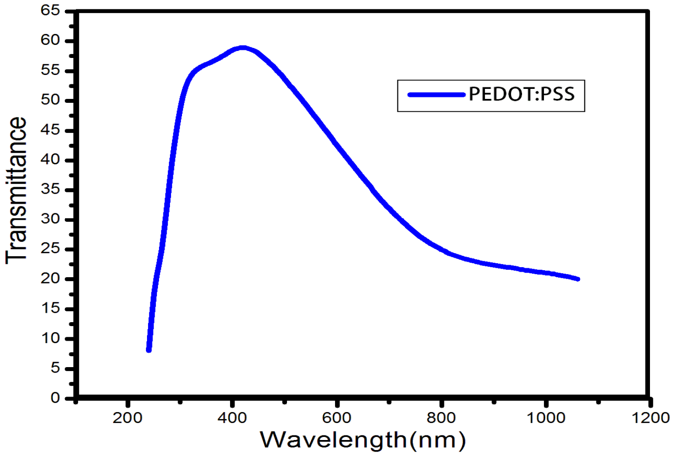

Figure 3.2: UV-visible transmittance spectra of the PEDOT: PSS under room temperature

The UV-VISIBLE measurement was carried on the PEDOT: PSS solution in the room temperature. The Absorbance spectra of PEDOT: PSS Solution was shown in the figure.

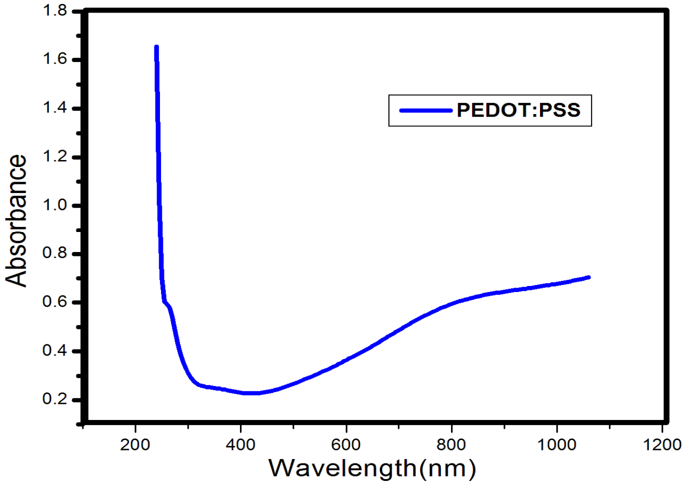

Figure 3.3: UV-visible absorption spectra of the PEDOT: PSS under room temperature.

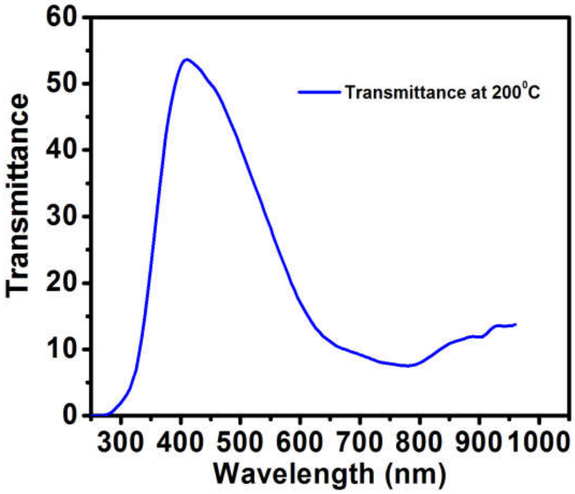

Figure 3.4: UV-visible Transmittance spectra of the MoO3 at 200 degree centigrade temperature.

3.2 Thickness measurement

In our lab currently we have variable angle spectroscopic ellipsometry whose model no is HO-SE-01 is an optical technique which is used for the measurement of film thickness. In this incident angle is equal to be Brewster angle. In our lab currently we have variable angle spectroscopic ellipsometry whose model no is HO-SE-01 is an optical technique. In that first of all the incident angle is taken equal to the Brewster angle then after that polarizer is set to be zero with the help of device setup then after that measurement takes place, then according to that analysis can be taken place such that choose the model that is molybdenum trioxide and ITO as well and then curve fitting takes place then after few minutes the thickness measured, the thickness of Molybdenum film is measured and it’s found to be around 12nm.

3.3 Effect of temperature

Firstly the UV-VISIBLE spectra of molybdenum solution taken in the room temperature then we will give the heating treatment to the molybdenum solution up to 200 degree centigrade then again the UV-VISIBLE spectra of molybdenum solution taken as the effect of temperature shows the peaks in the range 600-800um becomes much more evident it shows that this fascinating phenomenon may be attributed to free electron being trapped in oxygen vacancies in these p-moo3.

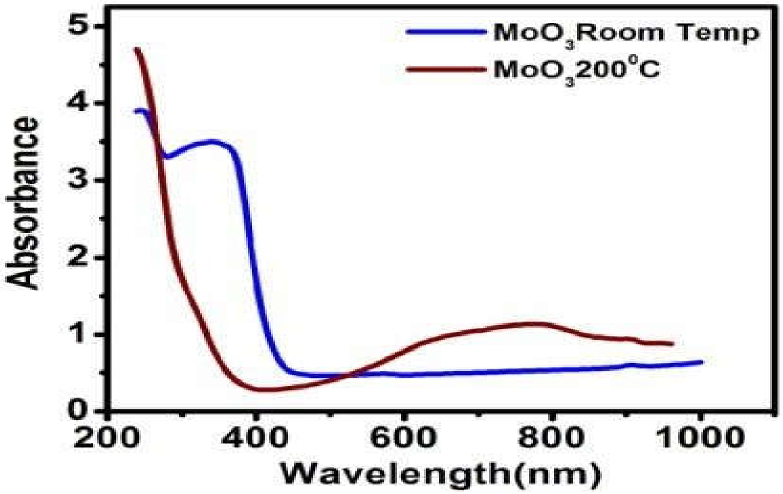

Figure 4. MoO3 at Room Temperature and 200 degree centigrade

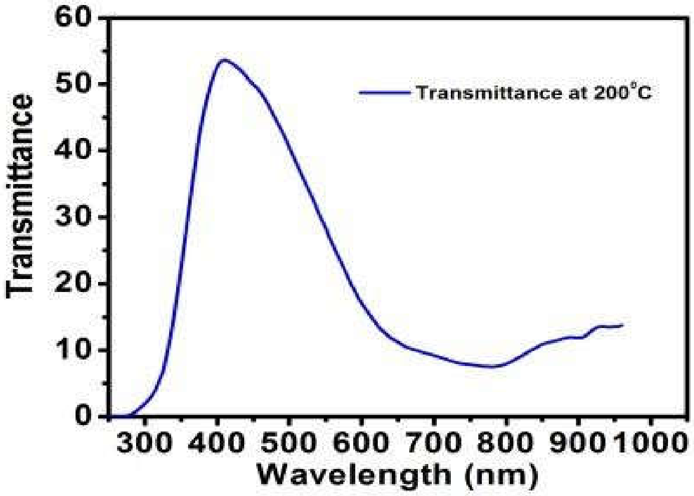

Figure 5. Transmittance of MoO3 at 200 degree centigrade.

4. Conclusions

The Molybdenum solution using Ethanediol and Isopropanol is synthesized by the treatment of the ultrasonic reaction. The characterization of the prepared p-MoO3 films were donefrom the spectroscopic measurement and SEM. It is found that the favorably smooth and dense surface morphology of the p-MoO3 layers are obtained under 200C with the good optical and electrical properties. Furthermore, the performance of the P3HT:PC71BM and PTB7:a PC71BM device with p-MoO3 thin films is found to depend strongly on the annealing and show best performance for 150 C. The improved performance of devices origin from the factors; (i) the favorable surface morphology of the annealed p-MoO3 films leading to higher rectification ratio and lower leakage current. (ii) The formation of oxygen vacancies and the growing Mo5+ cation leading to the change of WF under the annealing. Furthermore, the devices containing p-MoO3 thin film exhibited enhanced environmental stability. Overall, the simple and stable peroxomolybdic acid solution that we have developed is a viable candidate for replacing the PEDOT: PSS anode modifying layers in many organic solar cells including other electronic devices that require an ultrasmooth and high WF solution-processed hole selective contact.

References

1. Bernede, J. C. "Organic photovoltaic cells: history, principle and techniques." Journal of the Chilean Chemical Society 53.3 (2008): 1549-1564.
2. Lai, Tzung-Han, et al. "Properties of interlayer for organic photovoltaics." Materials Today 16.11 (2013): 424-432.
3. Hou, Jianhui, and Xia Guo. "Active layer materials for organic solar cells." OrganicSolar Cells. Springer London, 2013. 17-42.
4. Huei-Ting Chien, Markus Pölzl, Georg Koller, Susanna Challinger, Callum Fairbairn, Iain Baikie, Markus Kratzer, Christian Teichert, Bettina Friedel, Effects of hole-transport layer homogeneity in organic solar cells – A multi-length scale study, Surfaces and Interfaces, 2017,6, 72.
5. Ran Ji, Jiang Cheng, Xin Yang, Junsheng Yu, Lu Li, Enhanced charge carrier transport in spray-cast organic solar cells using solution processed MoO3micro arrays, RSC Adv., 2017, 7, 6, 3059.
6. Fei Cheng, Yiheng Wu, Yongcai Shen, Xueyuan CAI, Lingli Li, Enhancing the performance and stability of organic solar cells using solution processed MoO3 as hole transport layer, RSC Adv., 2017, 7, 60, 3795.
7. Haofan Sun, Quanqing Zhang, Lei Zhang, Weibing Zhang, Lingyi Zhang, Facile preparation of molybdenum (VI) oxide – modified graphene oxide nanocomposite for specific enrichment of phosphopeptides, Journal of Chromatography A, 2017.
8. Yanping Li, Huangzhong Yu, Xinxin Huang, Zuping Wu, Haihong Xu, Improved

performance for polymer solar cells using CTAB-modified MoO 3 as an anode buffer layer, Solar Energy Materials and Solar Cells, 2017, 171, 72.

9. Ran Ji, Ding Zheng, Chang Zhou, Jiang Cheng, Junsheng Yu, Lu Li, Low-Temperature Preparation of Tungsten Oxide Anode Buffer Layer via Ultrasonic SprayPyrolysis Method for Large-Area Organic Solar Cells, Materials, 2017, 10, 7, 820.

10. Yanping Li, Huangzhong Yu, Xinxin Huang, Zuping Wu, Mingdong Chen, A simple synthesis method to prepare a molybdenum oxide hole-transporting layer for efficient polymer solar cells, RSC Adv., 2017, 7, 13, 7890.

11. Hyoung Jin Son, Sung Hyun Kim, Dong Hwan Kim, Critical Impact of Hole Transporting Layers and Back Electrode on the Stability of Flexible Organic Photovoltaic Module, Advanced Energy Materials, 2017, 7, 5, 1601289.

12. Yanping Li, Xinxin Huang, “A simple synthesis method to prepare molybdenum oxide hole transport layer for efficient polymer solar cells, RSC Advances,2017.

13. Joseph Goldstein (2003). Scanning Electron Microscopy and X-Ray Microanalysis. Springer. ISBN 978-0-306-47292-3. Retrieved 26 May 2012.13

14. Siegfried Rebsdat; Dieter Mayer (2005), "Ethylene Glycol", Ullmann's Encyclopedia of Industrial Chemistry, Weinheim: Wiley-VCH, doi:10.1002/14356007.a10_10114

15. "Hydrogen peroxide". Immediately Dangerous to Life and Health. National Institute for Occupational Safety and Health (NIOSH).